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Control of Interface Evolution in Multi-Phase Fluid Flows: theory and computations

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joint work with: Ľ. Baňas (Edinburgh) and A. Prohl (Tübingen)

Oberseminar Numerik
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Outline

The Model

- $\rho_0 = \rho_1\chi_{\Omega_1} + \rho_2\chi_{\Omega_2}$ mixture of two immiscible viscous incompressible fluids in a bounded domain in $\mathbb{R}^2$.
- Multi-phase flow evolution by Navier–Stokes Eq. (cf. [Lions, 1996])

$$(NSE)\begin{cases} \rho\boldsymbol{y}_t + \rho[\boldsymbol{y}\cdot\nabla]\boldsymbol{y} - \mu\Delta\boldsymbol{y} + \nabla p = \rho\boldsymbol{u} + \rho\boldsymbol{g}, & \boldsymbol{y}(0) = \boldsymbol{y}_0, \\ \rho_t + [\boldsymbol{y}\cdot\nabla]\rho = 0, & \rho(0) = \rho_0, \\ \operatorname{div}\boldsymbol{y} = 0 & + B.C. \end{cases}$$

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The Model

Add additional term to functional to minimize the interface area!
$\Rightarrow$ Geometric functional!

$$\text{Minimize } J(\rho, \boldsymbol{u}) = \int_{\Omega_T} |\rho(t) - \sigma|^2 \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}t + \frac{\alpha}{2} \int_{\Omega_T} |\boldsymbol{u}|^2 \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}t + \frac{\beta}{2} \int_0^T \mathcal{H}^1(S_\rho) \, \mathrm{d}t$$

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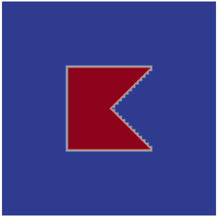
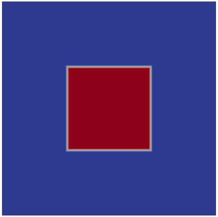
Evidence of the geometric functional

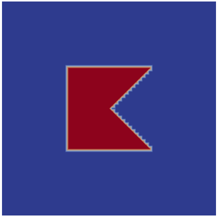
$\min \|\rho - \sigma\|^2_{L^2(\Omega_T)}$



Target σ



$\min \|\rho - \sigma\|^2_{L^2(\Omega_T)} + \int_0^T \mathcal{H}^1(S_\rho)$



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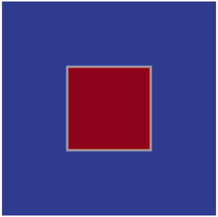

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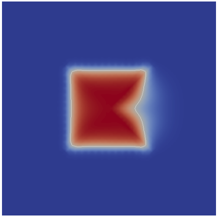

better corners

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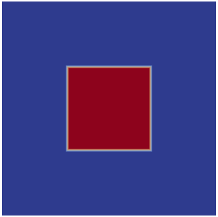

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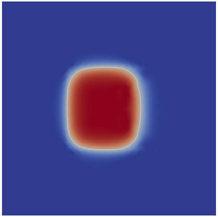
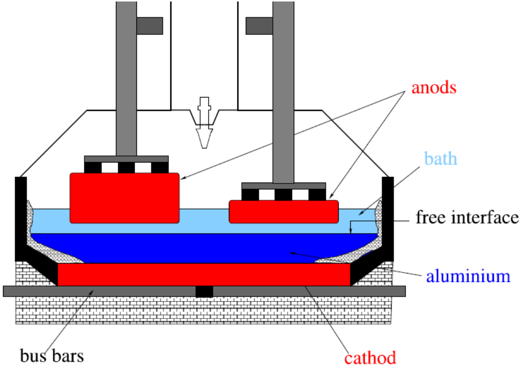


correct geometry

Application: Aluminium production



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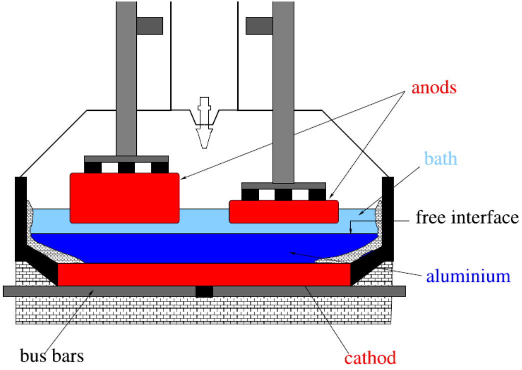
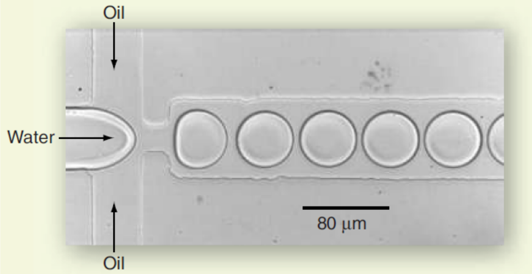


Anods shall not touch the interface! ⇒ Interface control ([Gerbeau et al., 2006])

Application: Droplet transport



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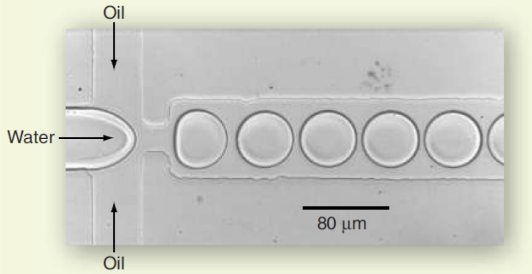

Control movement of droplets through a channel ⇒ Topology important ([Joanicot and Ajdari, 2005])

Goals

- Existence of optimum
- Optimality conditions
- Numerical scheme with low order Finite Elements
- Convergence of the numerical scheme

Known result

- Optimization (analysis, no numerics) of L^2-functional (no geometric term) subject to Stokes equation, cf. [Kunisch and Lu, 2011].
- Convergent numerical scheme for equation (low regularity), cf. [Baňas and Prohl, 2010].

Analytical problems and strategy

Minimize

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- **Problem:** Not clear if blue term is w.l.s.c., and not clear if corresponding Lagrange multiplier to mass equation exists and is a function.
- **Solution:** Add artificial diffusion to equation and approximate Hausdorff measure ("Mortola-Modica", cf. [Braides, 1998])

$\Rightarrow$ **Phase-field formulation**

Analytical problems and strategy

Minimize

$$J_\delta(\rho, \boldsymbol{u}) = \int_{\Omega_T} |\rho(t) - \sigma|^2 + \frac{\alpha}{2} \int_{\Omega_T} |\boldsymbol{u}|^2 + \frac{\beta}{2} \left(\delta \int_{\Omega_T} |\nabla \rho|^2 + \frac{1}{4\delta} \int_{\Omega_T} W(\rho) \right)$$

subject to

$$(NSE_\varepsilon) \begin{cases} \rho \boldsymbol{y}_t + \rho[\boldsymbol{y} \cdot \nabla]\boldsymbol{y} - \mu \Delta \boldsymbol{y} + \nabla p = \rho \boldsymbol{u} + \rho \boldsymbol{g}, & \boldsymbol{y}(0) = \boldsymbol{y}_0, \\ \rho_t + [\boldsymbol{y} \cdot \nabla]\rho - \varepsilon \Delta \rho_t = 0, & \rho(0) = \rho_0, \\ \operatorname{div} \boldsymbol{y} = 0 & + B.C. \end{cases}$$

($W \geq 0$ double Well functional with $W(\rho) = 0$ iff $\rho = \rho_1$ or $\rho = \rho_2$)

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Proof.

Lot of technical calculations. Key are a priori estimates and regularity:

- Use parabolic theory for regularity of ρ.
- Use [Lions, 1996] for regularity of $\boldsymbol{y}$.

Then direct application of Lagrange multiplier theorem. □

Passing to the limit for $\varepsilon, \delta \to 0$?

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- For $\delta \searrow 0$ (and no side constraints), it is known ([Braides, 1998]) that $J_\delta(\rho, \boldsymbol{u}) \xrightarrow{\Gamma} J(\rho, \boldsymbol{u})$ (Γ-convergence), i.e.,
  1. For every sequence $(\rho_\delta, \boldsymbol{u}_\delta) \to (\rho, \boldsymbol{u})$ (for $\delta \to 0$) we have
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Open question: How to combine both results? How to choose $\delta = \delta(\varepsilon)$?

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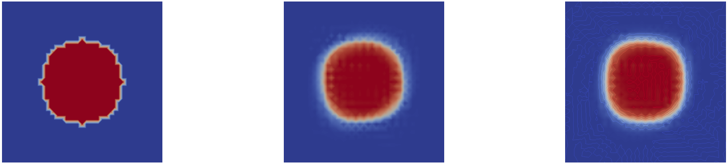
By a priori estimates, we have $\|\nabla \rho\|^2_{L^2(\Omega_T)} \leq \frac{1}{\varepsilon}$.

Guess: $\delta \approx \varepsilon$

Case $\varepsilon \ll \delta$: parasitic velocities

$\min \delta \int_{\Omega_T} |\nabla \rho|^2 + \frac{1}{4\delta} \int_{\Omega_T} W(\rho)$ s.t. (NSE_ε).



$\rho(t = 0)$ $\rho(t = 0.25)$ $\rho(t = 0.5)$

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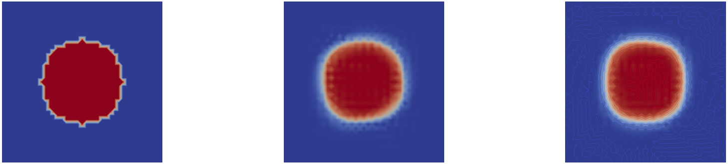

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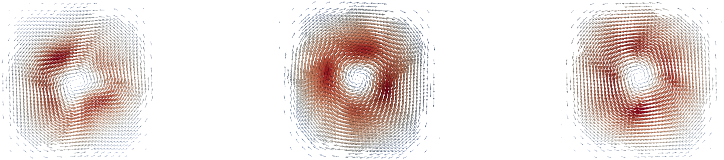
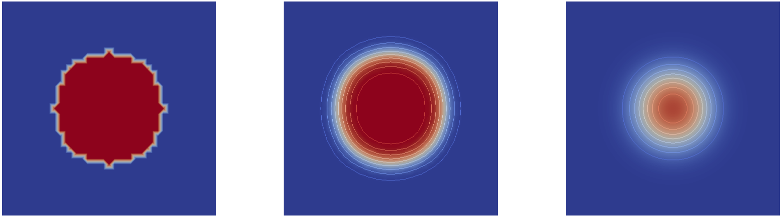


$\boldsymbol{y}(t=0.05)$ $\boldsymbol{y}(t=0.15)$ $\boldsymbol{y}(t=0.35)$

Case $\varepsilon \gg \delta$: massive diffusion

$$\min \delta \int_{\Omega_T} |\nabla \rho|^2 + \frac{1}{4\delta} \int_{\Omega_T} W(\rho) \text{ s.t. } (NSE_\varepsilon).$$



$\rho(t = 0)$ | $\rho(t = 0.5)$ moderate ε | $\rho(t = 0.5)$ big ε

Optimality Conditions

$$\mathbf{0} = \frac{1}{2}\eta\nabla\rho - \frac{1}{2}\rho\nabla\eta - \frac{1}{2}\rho_t\boldsymbol{z} - \rho\boldsymbol{z}_t + \frac{1}{2}\rho\nabla\boldsymbol{y}\boldsymbol{z} - \frac{1}{2}[\nabla\rho\cdot\boldsymbol{y}]\boldsymbol{z}$$
$$- \rho[\boldsymbol{y}\cdot\nabla]\boldsymbol{z} - \frac{1}{2}\rho\nabla\boldsymbol{z}\boldsymbol{y} - \mu\Delta\boldsymbol{z} - \nabla q,$$
$$0 = \operatorname{div}\boldsymbol{z}, \operatorname{div}\boldsymbol{y}$$
$$0 = \lambda(\rho - \tilde{\rho}) - \beta\delta\Delta\rho + \frac{\beta}{8\delta}W'(\rho) - \eta_t - [\boldsymbol{y}\cdot\nabla]\eta + \varepsilon\Delta\eta_t$$
$$+ \frac{1}{2}\boldsymbol{z}\cdot\boldsymbol{y}_t - \frac{1}{2}\boldsymbol{y}\cdot\boldsymbol{z}_t + \frac{1}{2}[\boldsymbol{y}\cdot\nabla]\boldsymbol{y}\cdot\boldsymbol{z} - \boldsymbol{u}\cdot\boldsymbol{z} - \frac{1}{2}[\boldsymbol{y}\cdot\nabla]\boldsymbol{z}\cdot\boldsymbol{y},$$
$$\mathbf{0} = \alpha\boldsymbol{u} - \rho\boldsymbol{z},$$
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$\boldsymbol{z}(T) = \mathbf{0}$, $\eta(T) = 0$ + B.C.

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\begin{aligned}
\mathbf{0} &= \frac{1}{2}\eta\nabla\rho - \frac{1}{2}\rho\nabla\eta - \frac{1}{2}\rho_t\boldsymbol{z} - \rho\boldsymbol{z}_t + \frac{1}{2}\rho\nabla\boldsymbol{y}\boldsymbol{z} - \frac{1}{2}[\nabla\rho\cdot\boldsymbol{y}]\boldsymbol{z} \\
&\quad - \rho[\boldsymbol{y}\cdot\nabla]\boldsymbol{z} - \frac{1}{2}\rho\nabla\boldsymbol{z}\boldsymbol{y} - \mu\Delta\boldsymbol{z} - \nabla q, \\
0 &= \operatorname{div}\boldsymbol{z}, \operatorname{div}\boldsymbol{y} \\
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Strategy for discretization

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- Due to strong coupling of primal and dual variables in the adjoint equation, we need bounds on higher bounds of the primal variables.
- Here: Fix $\delta, \varepsilon > 0$. Still open: Interplay between δ, ε and numerical parameters (time step size k and grid size h)?

Numerical framework

- Density space R_h: standard piecewise linear FE space.
- Velocity/pressure space $\boldsymbol{V}_h/M_h$: standard inf-sup-stable FE spaces (e.g., Taylor–Hood).
- Time discretization: (Semi)Implicit Euler.

Find $(\boldsymbol{Y}^n, P^n, R^n) \in \boldsymbol{V}_h \times M_h \times R_h$ such that for all $(\boldsymbol{Z}, \Pi, E) \in \boldsymbol{V}_h \times M_h \times R_h$:

$$
\begin{aligned}
(d_t R^n, E) + \varepsilon(d_t \nabla R^n, \nabla E) + ([\boldsymbol{Y}^n \cdot \nabla] R^n, E) + \frac{1}{2}(R^n \operatorname{div} \boldsymbol{Y}^n, E) &= 0, \\
\frac{1}{2}(R^{n-1} d_t \boldsymbol{Y}^n, \boldsymbol{Z}) + \frac{1}{2}(d_t(R^n \boldsymbol{Y}^n), \boldsymbol{Z}) + \frac{1}{2}([R^{n-1} \boldsymbol{Y}^{n-1} \cdot \nabla] \boldsymbol{Y}^n, \boldsymbol{Z}) & \\
- \frac{1}{2}([R^{n-1} \boldsymbol{Y}^{n-1} \cdot \nabla] \boldsymbol{Z}, \boldsymbol{Y}^n) + \mu(\nabla \boldsymbol{Y}^n, \nabla \boldsymbol{Z}) + (\nabla P^n, \boldsymbol{Z}) &= (R^{n-1} \boldsymbol{U}^n, \boldsymbol{Z}), \\
(\operatorname{div} \boldsymbol{Y}^n, \Pi) &= 0.
\end{aligned}
$$

Comments

Scheme is modification of scheme in [Baňas and Prohl, 2010].

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First line becomes skew symmetric.

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$$-\frac{1}{2}([R^{n-1} \boldsymbol{Y}^{n-1} \cdot \nabla] \boldsymbol{Z}, \boldsymbol{Y}^n) + \mu(\nabla \boldsymbol{Y}^n, \nabla \boldsymbol{Z}) + (\nabla P^n, \boldsymbol{Z}) = (R^{n-1} \boldsymbol{U}^n, \boldsymbol{Z}),$$

$$(\operatorname{div} \boldsymbol{Y}^n, \Pi) = 0.$$

Comments

Second line becomes skew symmetric as (cf. [Liu and Walkington, 2007])

$$\rho(\boldsymbol{y}_t + [\boldsymbol{y} \cdot \nabla] \boldsymbol{y}) = \frac{1}{2}\Big(\rho \boldsymbol{y}_t + \rho[\boldsymbol{y} \cdot \nabla] \boldsymbol{y} + (\rho \boldsymbol{y})_t + \operatorname{div}(\rho \boldsymbol{y} \otimes \boldsymbol{y})\Big).$$

Find $(\boldsymbol{Y}^n, P^n, R^n) \in \boldsymbol{V}_h \times M_h \times R_h$ such that for all $(\boldsymbol{Z}, \Pi, E) \in \boldsymbol{V}_h \times M_h \times R_h$:

$$(d_t R^n, E) + \varepsilon(d_t \nabla R^n, \nabla E) + ([\boldsymbol{Y}^n \cdot \nabla] R^n, E) + \frac{1}{2}(R^n \operatorname{div} \boldsymbol{Y}^n, E) = 0,$$

$$\frac{1}{2}(R^{n-1} d_t \boldsymbol{Y}^n, \boldsymbol{Z}) + \frac{1}{2}(d_t(R^n \boldsymbol{Y}^n), \boldsymbol{Z}) + \frac{1}{2}([R^{n-1} \boldsymbol{Y}^{n-1} \cdot \nabla] \boldsymbol{Y}^n, \boldsymbol{Z}) - \frac{1}{2}([R^{n-1} \boldsymbol{Y}^{n-1} \cdot \nabla] \boldsymbol{Z}, \boldsymbol{Y}^n) + \mu(\nabla \boldsymbol{Y}^n, \nabla \boldsymbol{Z}) + (\nabla P^n, \boldsymbol{Z}) = (R^{n-1} \boldsymbol{U}^n, \boldsymbol{Z}),$$

$$(\operatorname{div} \boldsymbol{Y}^n, \Pi) = 0.$$

Comments

Assume: Triangulation is strongly acute (iff angles of interior edges are bdd away from 90°)

$\Rightarrow$ M-matrix property for first line

$\Rightarrow$ lower bound for R^n

Lemma (Bounds for primal variables)

There exists a solution $\{(R^n, \boldsymbol{Y}^n, P^n)\}$ of the discrete equation with the property

$$0 < \rho_1 \leq R^n \leq C < \infty$$

and for the time interpolant of the solution $(\mathcal{R}, \boldsymbol{\mathcal{Y}}, \mathcal{P})$ there is a constant $C = C(\varepsilon, \delta, T)$ independent of k, h with

$$\sup_{t\in[0,T]} \left[\|\nabla \boldsymbol{\mathcal{Y}}(t)\|^2 + \|\Delta_h \mathcal{R}(t)\|^2\right] + \int_0^T \|\Delta_h \boldsymbol{\mathcal{Y}}(t)\|^2 + \|d_t \boldsymbol{\mathcal{Y}}(t)\|^2 + \|d_t \nabla \mathcal{R}(t)\|^2 \, \mathrm{d}t \leq C.$$

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Proof.

Test equations with $\boldsymbol{Y}^n$ and R^n, resp.

□

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Proof.

Test mass equation with $-\Delta_h R^n$.

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Proof.

Test mass equation with $-\Delta_h d_t R^n$

□

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Proof.

Test momentum equation with $d_t \boldsymbol{Y}^n$ and Stokes operator $\boldsymbol{A}_h \boldsymbol{Y}^n$ simultaneously. □

Discrete Optimality Conditions

$$
\begin{aligned}
0 =\ & \frac{1}{2}E^n\nabla R^n - \frac{1}{2}R^n\nabla E^n - \frac{1}{2}d_t R^n \boldsymbol{Z}^n - R^n d_t \boldsymbol{Z}^{n+1} + \frac{1}{2}R^n\nabla \boldsymbol{Y}^{n+1}\cdot \boldsymbol{Z}^{n+1} \\
& + \frac{1}{2}R^n\nabla \boldsymbol{Z}^{n+1}\cdot \boldsymbol{Y}^{n+1} - \frac{1}{2}(\nabla R^{n-1}\cdot \boldsymbol{Y}^{n-1})\boldsymbol{Z}^n - \frac{1}{2}R^{n-1}\operatorname{div}\boldsymbol{Y}^{n-1}\boldsymbol{Z}^n \\
& - \frac{1}{2}[R^{n-1}\boldsymbol{Y}^{n-1}\cdot\nabla]\boldsymbol{Z}^n - \mu\Delta_h \boldsymbol{Z}^n - \nabla Q^n, \\
0 =\ & -\operatorname{div}\boldsymbol{Z}^n, \\
0 =\ & -d_t E^{n+1} - [\boldsymbol{Y}^n\cdot\nabla]E^n - \frac{1}{2}(\operatorname{div}\boldsymbol{Y}^n)E^n + \varepsilon d_t\Delta_h E^{n+1} + \frac{1}{2}d_t\boldsymbol{Y}^{n+1}\cdot\boldsymbol{Z}^{n+1} \\
& - \frac{1}{2}\boldsymbol{Y}^n\cdot d_t\boldsymbol{Z}^{n+1} + \frac{1}{2}[\boldsymbol{Y}^n\cdot\nabla]\boldsymbol{Y}^{n+1}\cdot\boldsymbol{Z}^{n+1} - \boldsymbol{U}^{n+1}\cdot\boldsymbol{Z}^{n+1} \\
& - \frac{1}{2}[\boldsymbol{Y}^n\cdot\nabla]\boldsymbol{Z}^{n+1}\cdot\boldsymbol{Y}^{n+1} + \lambda(R^n - \tilde{\rho}(t_n)) - \beta\delta\Delta_h R^n + \frac{\beta}{8\delta}W'(R^n), \\
0 =\ & \alpha\boldsymbol{U}^n - R^{n-1}\boldsymbol{Z}^n.
\end{aligned}
$$

Lemma (Bounds for dual variables)

By the Lagrange multiplier theorem, there exist Lagrange multipliers $(\mathcal{Z}, \mathcal{Q}, \mathcal{E})$ and there exists a constant $C = C(\varepsilon, \delta, T)$ independent of k, h with

$$\sup_{t\in[0,T]} \left[\|\nabla\mathcal{E}\|^2 + \|\mathcal{Z}\|^2\right] + \int_0^T \|\nabla\mathcal{Z}\|^2 + \|d_t\mathcal{Z}\|^2 \,\mathrm{d}t \leq C.$$

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Proof.

Simultaneously test discrete optimality system with $\boldsymbol{Z}^n$, E^n and $d_t\boldsymbol{Z}^{n+1}$. □

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Theorem (Convergence)

There exist $\boldsymbol{y}, p, \rho; \boldsymbol{z}, q, \eta; \boldsymbol{u} : \Omega_T \to \mathbb{R}^{(2)}$, such that the solutions of the fully discrete optimality system converge to them in some norms (up to subsequences). The limit functions solve the original fully continuous optimality system.

Computational framework

1. Use Taylor–Hood Finite Elements for velocity and pressure.

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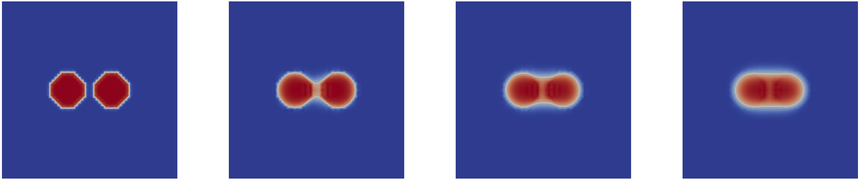
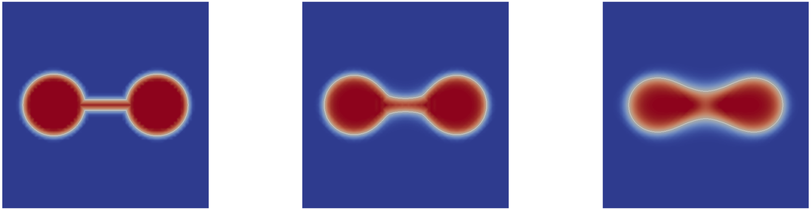
2. Use gradient algorithm for discrete optimality conditions
3. Observation: Regularization of mass equation with $-\Delta\rho$ works fine. No need to insert time derivative. In this case, we also have $0 < \rho_1 \leq R^n \leq \rho_2 < \infty$.

$$\min \int_0^T \mathcal{H}^1(S_\rho)$$



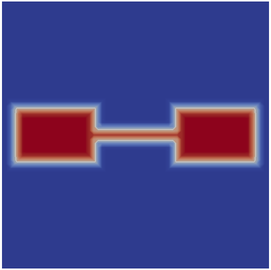
$\rho(t = 0)$ $\rho(t = 0.15)$ $\rho(t = 0.5)$ $\rho(t = 1)$

$$\min \int_0^T \mathcal{H}^1(S_\rho)$$



$\rho(t = 0)$ $\rho(t = 0.15)$ $\rho(t = 1)$

$$\min \int_0^T \mathcal{H}^1(S_\rho)$$



$$\rho(t=0)$$

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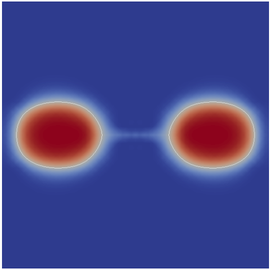
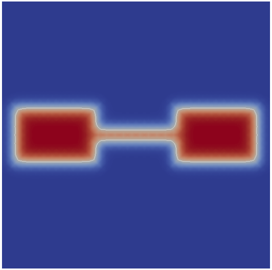


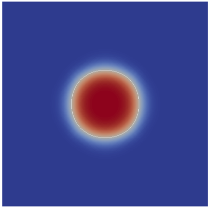
$\rho(t = 1)$

Control $u \equiv 0$

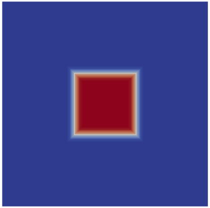


$\rho(t = 1)$

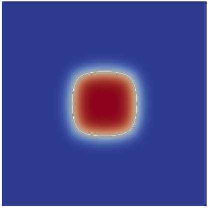
$\min \int_0^T \mathcal{H}^1(S_\rho)$



Target σ



$\min \int_0^T \mathcal{H}^1(S_\rho)$
$+\|\rho - \sigma\|^2_{L^2(\Omega_T)}$



In a nutshell

$$J(\rho, \boldsymbol{u}) = \int_{\Omega_T} |\rho(t) - \sigma|^2 \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}t + \frac{\beta}{2} \int_0^T \mathcal{H}^1(S_\rho) \, \mathrm{d}t + \frac{\alpha}{2} \int_{\Omega_T} |\boldsymbol{u}|^2 \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}t$$

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- When shape is important, use β small

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- When shape is important, use β small
- When topology is important and target has “good” topology, use β big.

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$$J(\rho, \boldsymbol{u}) = \int_{\Omega_T} |\rho(t) - \sigma|^2 \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t + \frac{\beta}{2} \int_0^T \mathcal{H}^1(S_\rho)\,\mathrm{d}t + \frac{\alpha}{2} \int_{\Omega_T} |\boldsymbol{u}|^2 \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t$$

- When shape is important, use β small
- When topology is important and target has “good” topology, use β big.

Play with balance of the first two terms!

Done

- Existence for optimization of geometric functional for $\delta, \varepsilon > 0$.
- Optimality conditions for $\delta, \varepsilon > 0$.
- Discretization of optimality conditions.
- Convergence analysis with unconditionally stable scheme.

Outlook

- What happens for $\varepsilon, \delta \to 0$?
- Compare model with corresponding models like the graph formulation, thin film equation, etc.
- Surface tension?

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THANK YOU FOR YOUR ATTENTION!

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